COMBUSTION LABORATORIES
THE UNIVERSITY OF ALABAMA
LOW EMISSIONS • HIGH EFFICIENCY • FUEL FLEXIBILITY

Characterization of Biomass-Based Fuels and Fuel Blends for Low-Emissions, Advanced Compression Ignition Engines (Co-Optima)

Ajay Agrawal (PI), Joshua Bittle,
The University of Alabama

June 20, 2018

Project ID: FT062

THE UNIVERSITY OF ALABAMA

Overview

Timeline

- Project start date: Feb 1, 2017
- Project end date: Jan 31, 2020
- Percent complete: 35%

Budget

- Total project funding
  - $630,493
  - DOE share: $567,301
  - Cost share: $63,192
- Funding received in FY 2017
  - $198,252
- Funding for FY 2018
  - $180,642

Barriers

- Co-optimization of fuels and engines
- Lack of fundamental knowledge of advanced engine combustion regimes
- Lack of effective engine controls

Partners

- Sandia National Laboratory
- Argonne National Laboratory

Project Objectives

Experimental Goal:

- Acquire repeatable fuel-air mixing and combustion data using a constant pressure flow rig (CPFR)
- Implement multiple time-resolved optical diagnostics techniques simultaneously at diesel operating temperatures and pressures.
- Acquire experimental measurements to determine combustion properties of biofuels and blends
- Facilitate leaner lifted flame combustion in ACI engines.

Modeling Goal:

- Develop correlations between fuel properties and combustion properties
- Eventually develop a neural network based fuel property prediction tool for ACI engines.

<u>Address Sub-topic Area 1: Fuel Characterization and Fuel Property Prediction</u>

Project Approach

- **Experiment Setup and Measurement Processing Development:** Initial diagnostic integration into the existing constant pressure flow rig (CFR) as well as development of the data processing techniques will be completed. Additionally, assessment of potential modeling approaches (functional relations versus neural network) will be conducted.

- **Single component fuel testing and model development:** Single component fuel experiments and model development based on initial survey will be completed. Specific experimental conditions (and fuels) will be chosen based on discussions with DOE National Lab partner.

- **Multi-component fuel testing and blending rule development:** Experiments and blending models for multicomponent fuels will be completed. Finally, the tools developed will be used to identify a preliminary candidate fuel optimized for use in ACI engines.

Milestones

2017 Milestone	Type	Description
Optical Setup Complete	Technical	The existing spray chamber will be augmented with the additional diagnostics, chemiluminescence and two-color pyrometry, and the data capture synchronized.
Fuel Property Combustion Indicators Identified	Technical	Identified potential fuel properties to test for relation to combustion properties. This includes supercritical fuel property effects.
Image Processing Codes Complete	Technical	Completed development of image processing codes to provide synchronized spatial and temporal measurements.
Modelling approach decision	Go/No Go	Decision between functional model and neural network will be made at end of Budget Period 1. This will guide model development in remainder of project.

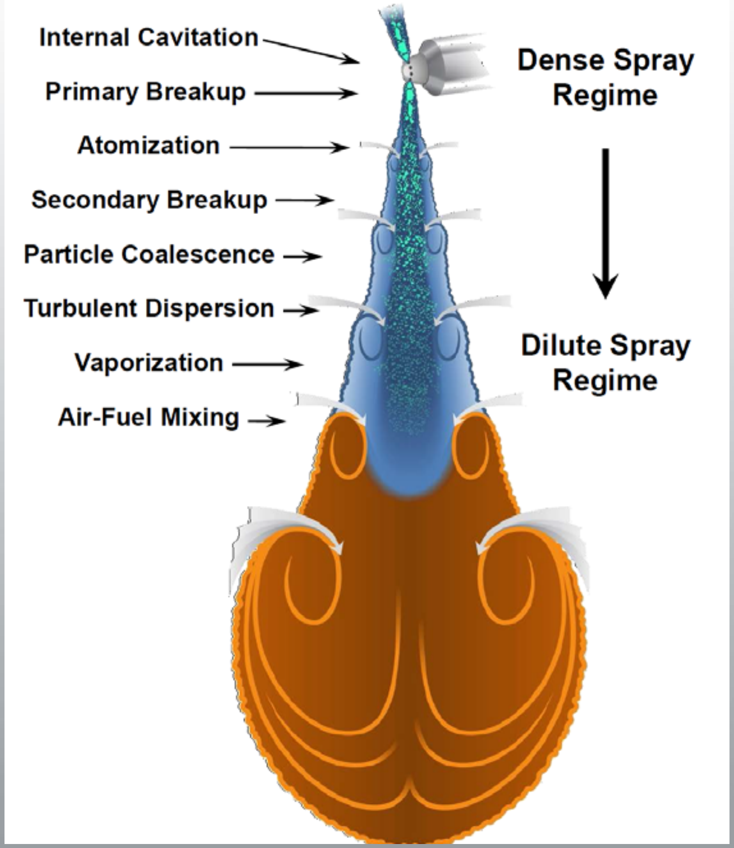
2018 Milestone	Type	Description
Initial Model Structure Developed	Technical	Based on fuel properties and combustion properties and initial model structure will be completed
Completed Single Fuel Testing	Technical	Spray tests of single component fuels will be completed to support model development
Petroleum based fuel models created	Technical	Models for single component petroleum based fuels will be created
Single Fuel Models Completed	Go/No Go	Single component combustion property models (petroleum and bio based) completed with acceptable accuracy

Project Accomplishments

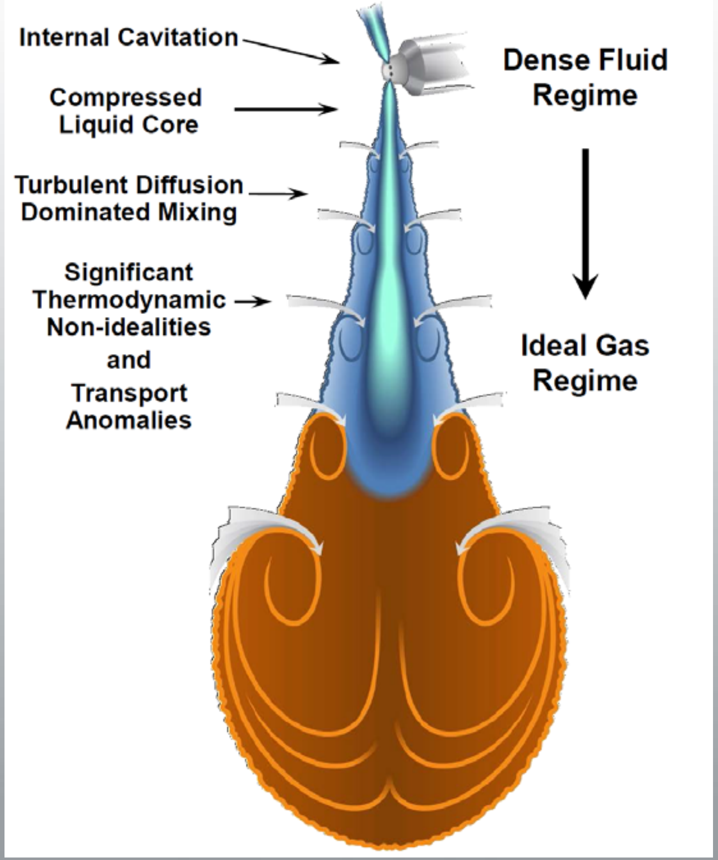
- Obtained baseline measurements in Constant Pressure Flow Rig for a baseline conditions using Rainbow Schlieren Deflectometry (RSD) Technique, and developed data processing techniques.
- Developed a two-color pyrometry system, and associated calibration and image processing techniques
- Tested time-resolved OH* chemiluminescence system, and developed imaging processing techniques
- Integrated the three diagnostics systems for simultaneous use in the constant pressure flow rig (CPFR)
- Evaluated functional model and neural network model approaches and decided to pursue neutral network model approach.
- Developed a trial neural network model for liquid penetration length using ECN experimental dataset.

Differing Spray Regimes

Conventional, Subcritical Processes



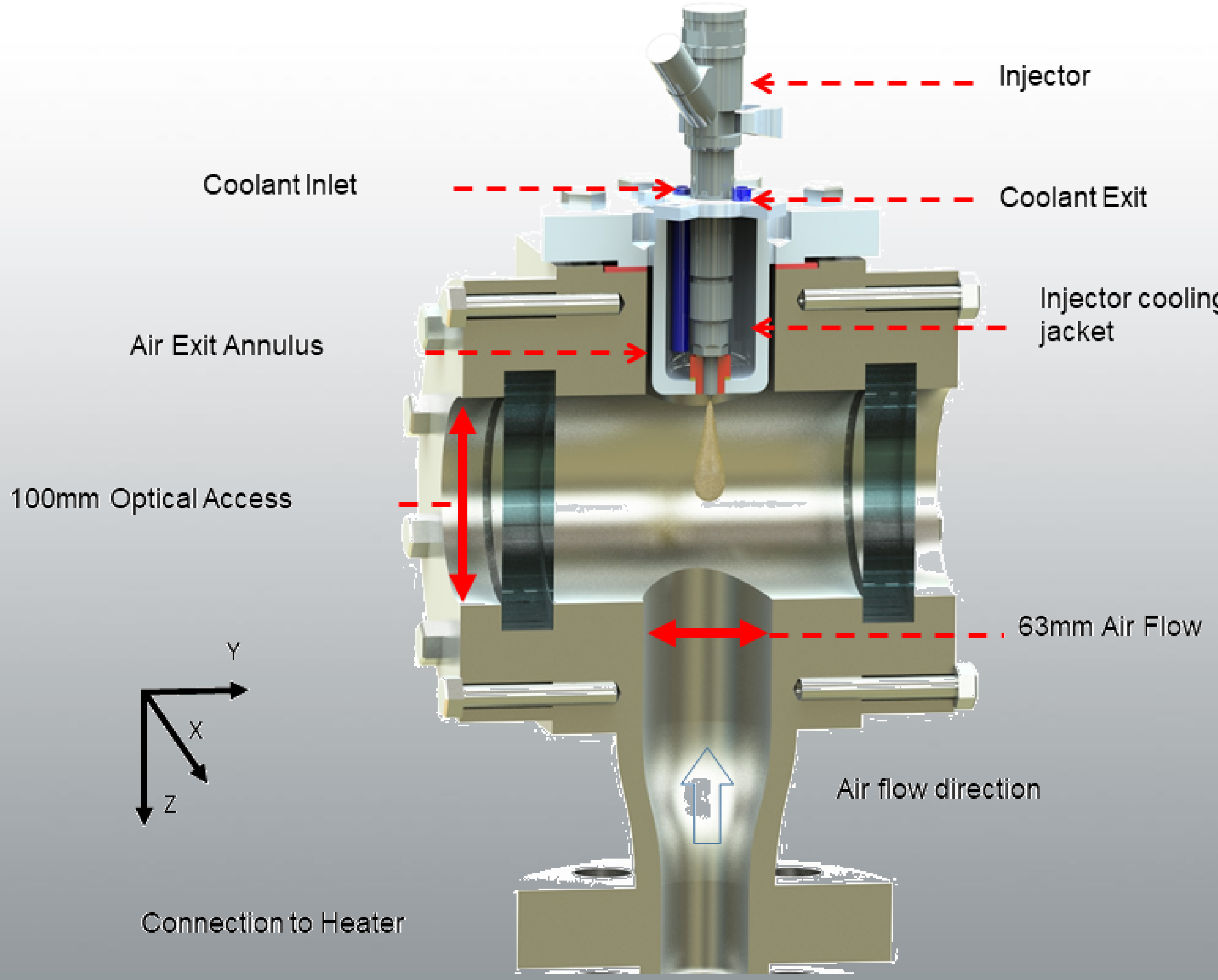
Supercritical Processes

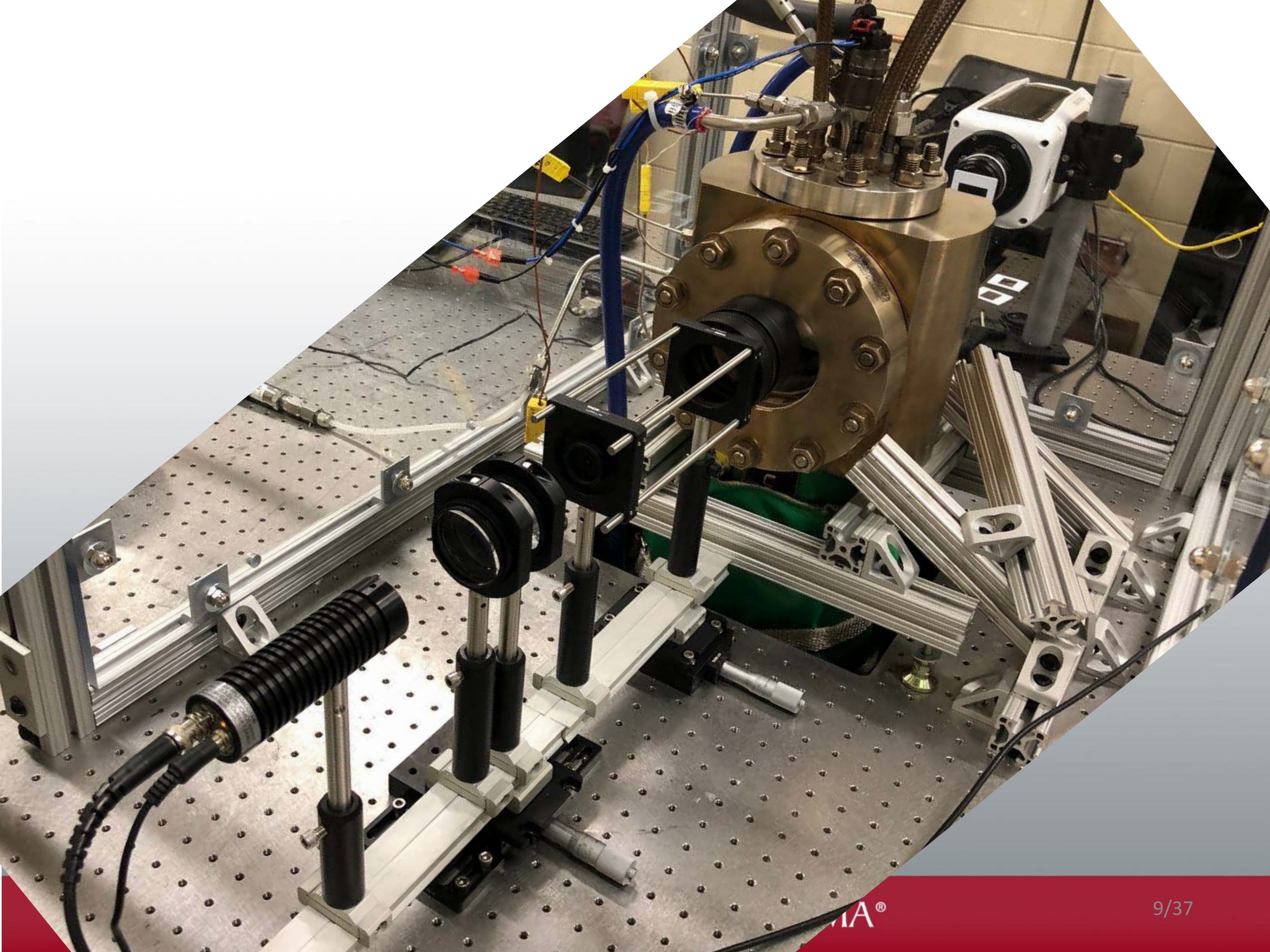


Oefelein, et al, AEC Update 2012

Constant Pressure Flow Rig (CPFR)

- Continuous flow of compressed preheated air
- Bosch CRIN3-18 Injector, axial 100 µm orifice
- 12 injections per minute

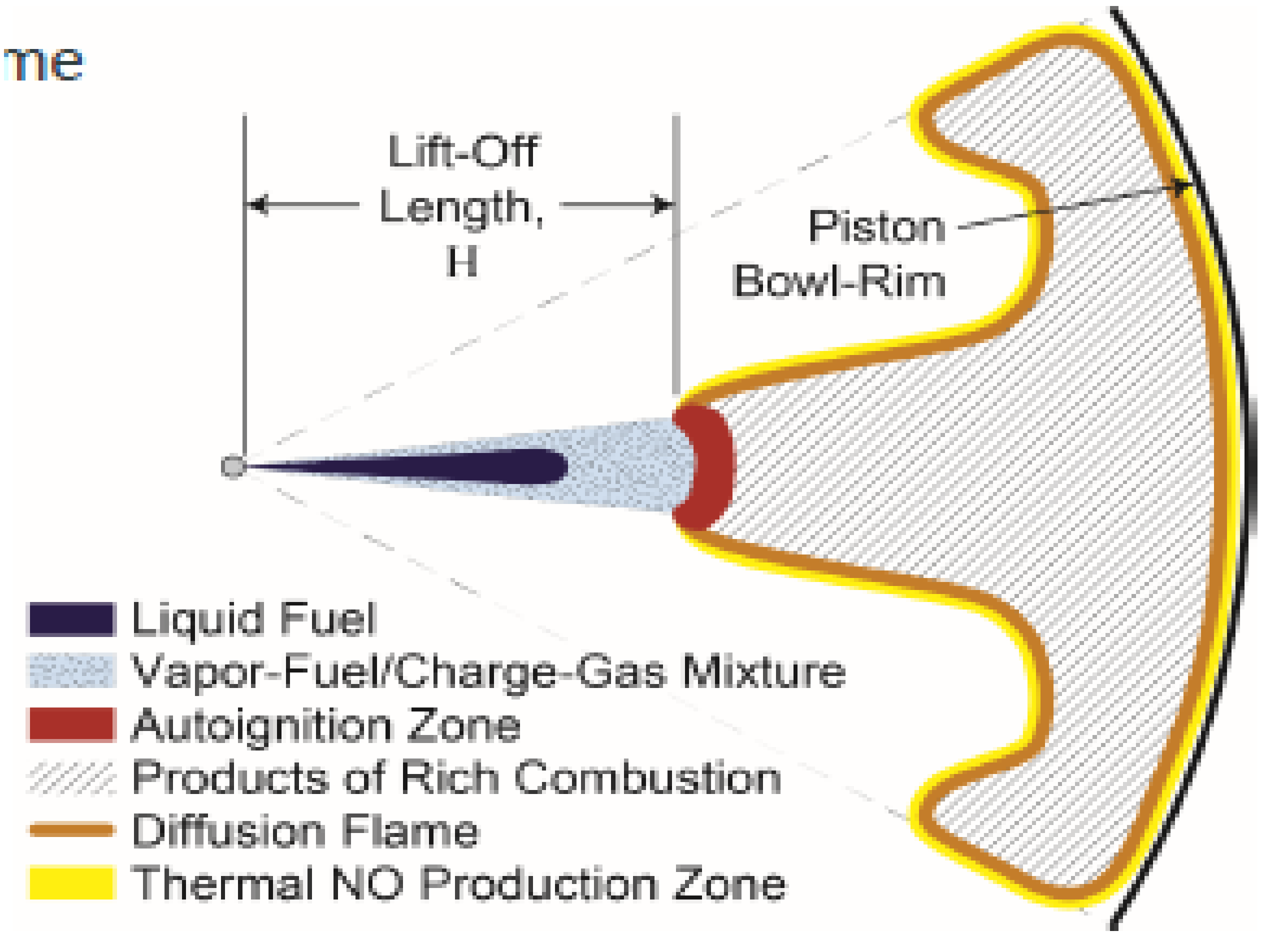




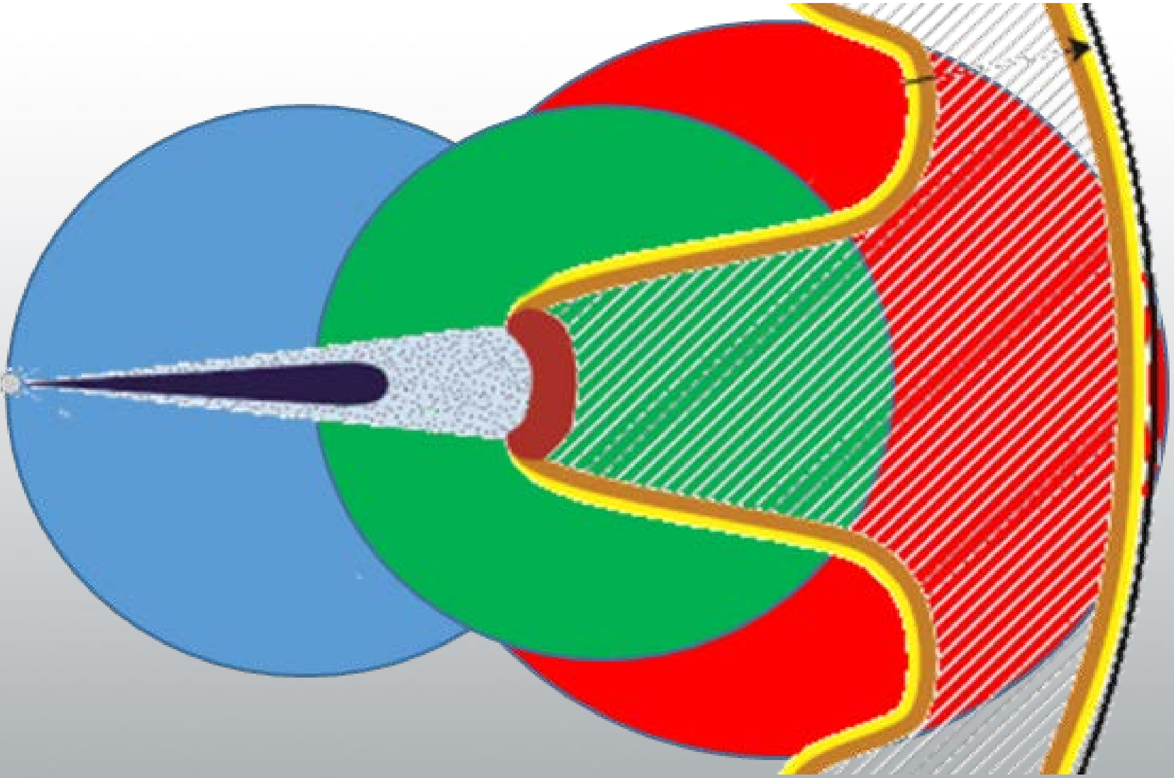
Lean Lifted Flame Combustion

:ios ≤ 2

me



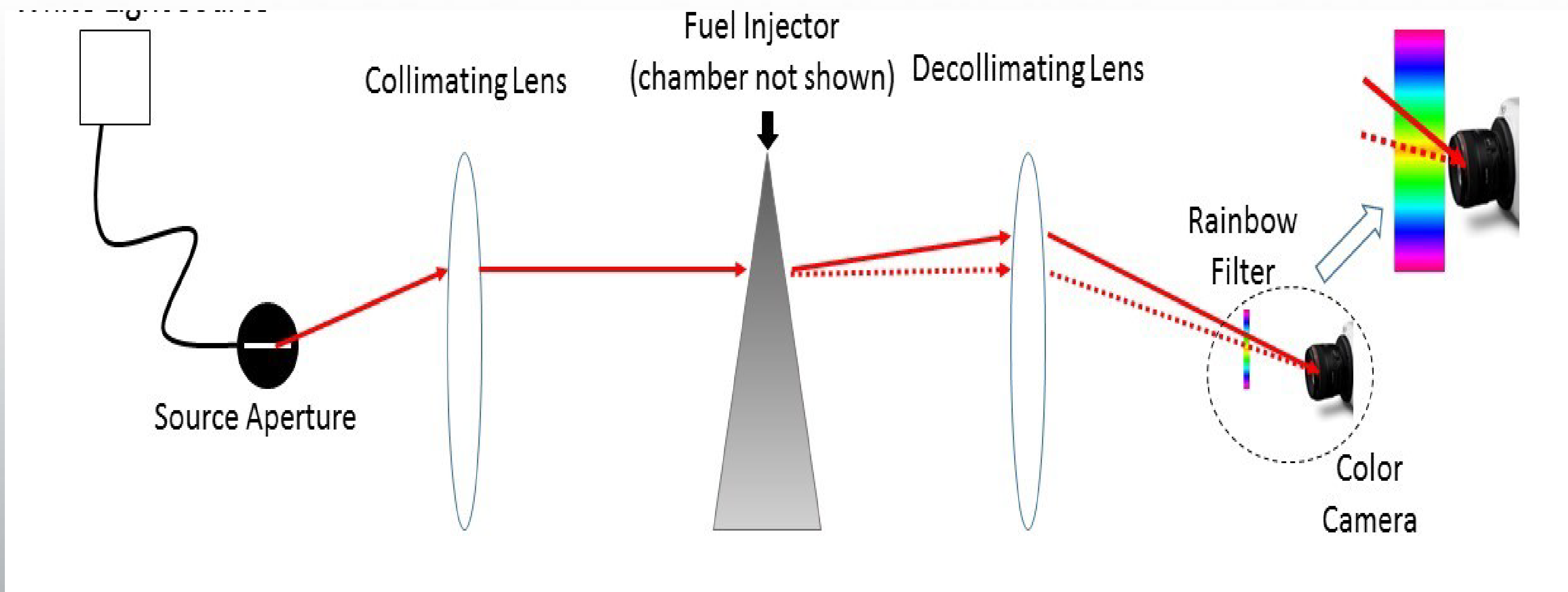
Optical Diagnostics



Diagnostics applied to lean lifted flame showing regions of imaging for Rainbow Schlieren Deflectometry or RSD (blue), OH (Green), and two-color pyrometer (red).*

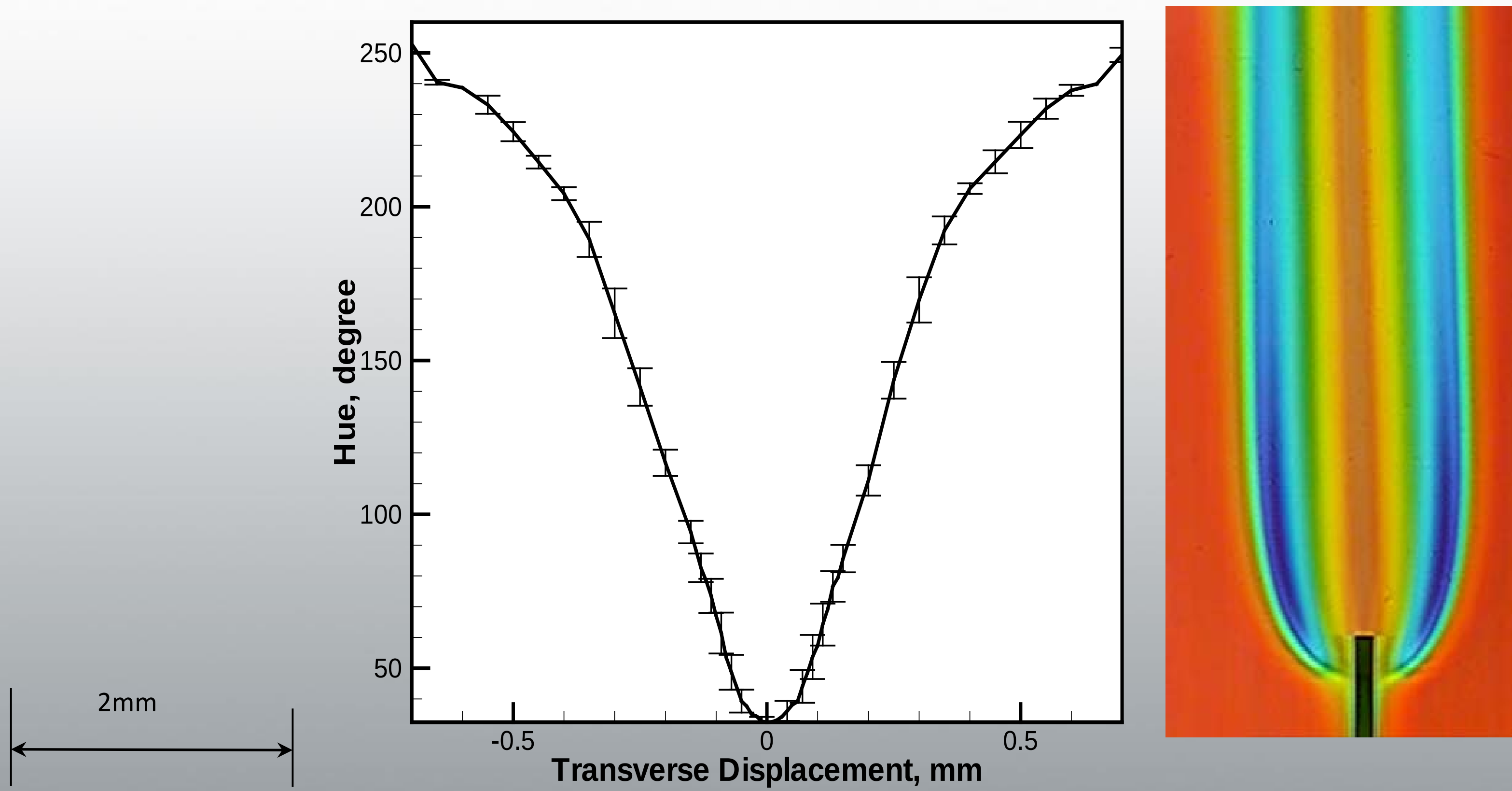
Rainbow Schlieren Deflectometry (RSD)

Pulsed Broadband LED



- High-intensity, pulsed LED white light source, rectangular source aperture, collimating and decollimating lenses
- Rainbow filter, high-speed camera

Rainbow Schlieren Deflectometry



(a) **(b)** **(c)**

Rainbow filter serves as an optical ruler to measure ray displacement

Test Conditions

– n-heptane
– Fuel supply pressure of 1000 bar
– Chamber air temperature of 825 K ($T_{f,cr}$ = 540 K)
– Chamber pressure of 28 bar ($P_{f,cr}$ = 27.4 bar)
– Schlieren field of view is about 60 mm
– Imaging Setup (Phantom v611)
  - Exposure time: 4 us
  - Framing rate: 40 kHz
  - Spatial resolution 100 um/px

Sample High-speed Video Imaging

These results are captured with small backlight on injector and liquid region.

780 K, 33 bar ambient conditions.

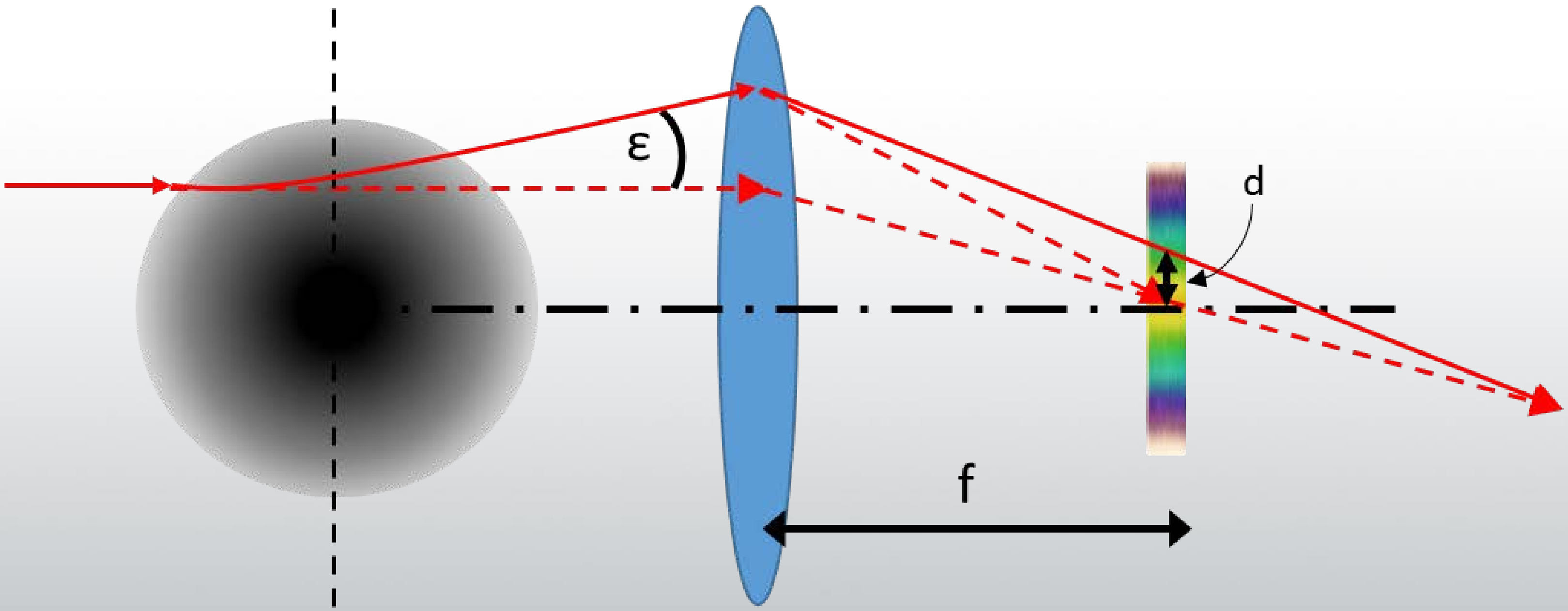
Injection duration (visual) = 2.6 ms
Main Ignition delay = 1.9 ms

RSD Video

Injection Duration (from video) = 4.75 ms

1st Stage ignition Delay = 0.65 ms, Main Ignition Delay = 1.0 ms

Schlieren Analysis



Instantaneous radial deflection angle at a transverse location 'x' is given as

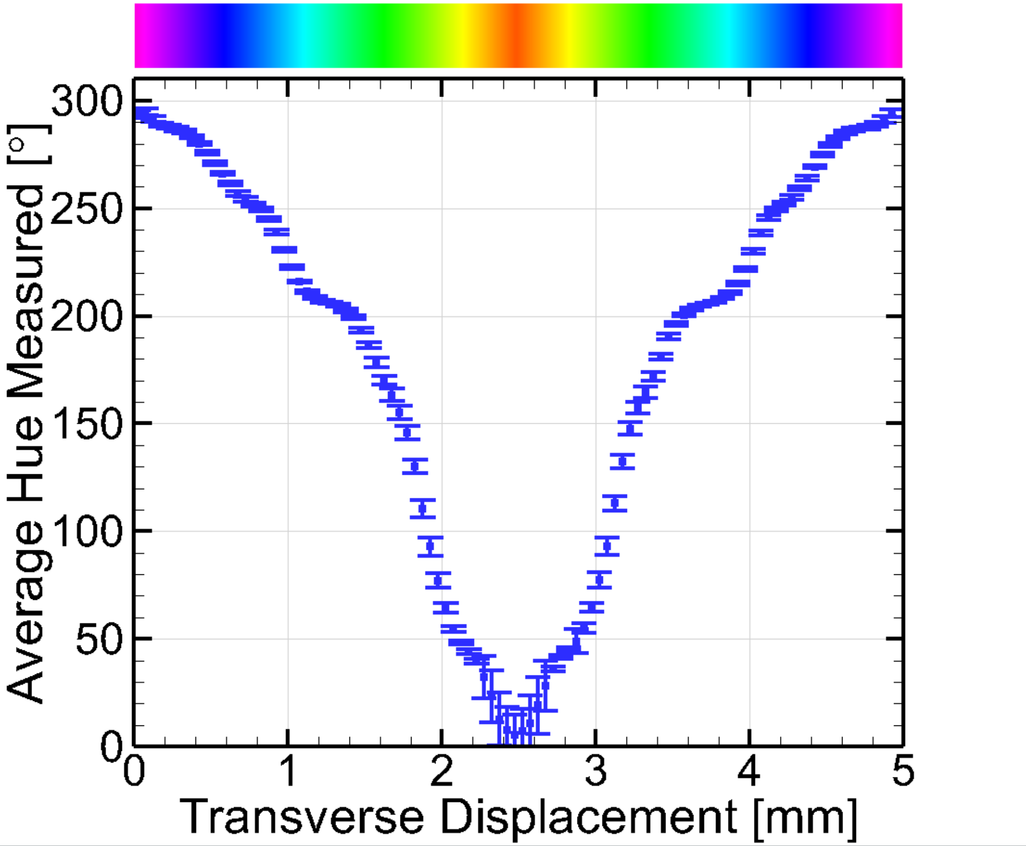
$$\varepsilon(x,t) = \int \frac{\partial \delta}{\partial x}(x,y,t)dy$$

Where $\delta = (\frac{n}{n_o} - 1)$ is the normalized refractive index difference, n is local refractive index, and n_o is ambient refractive index.

For small deflection angles, $\varepsilon(x,t)$=d(x,t)/f

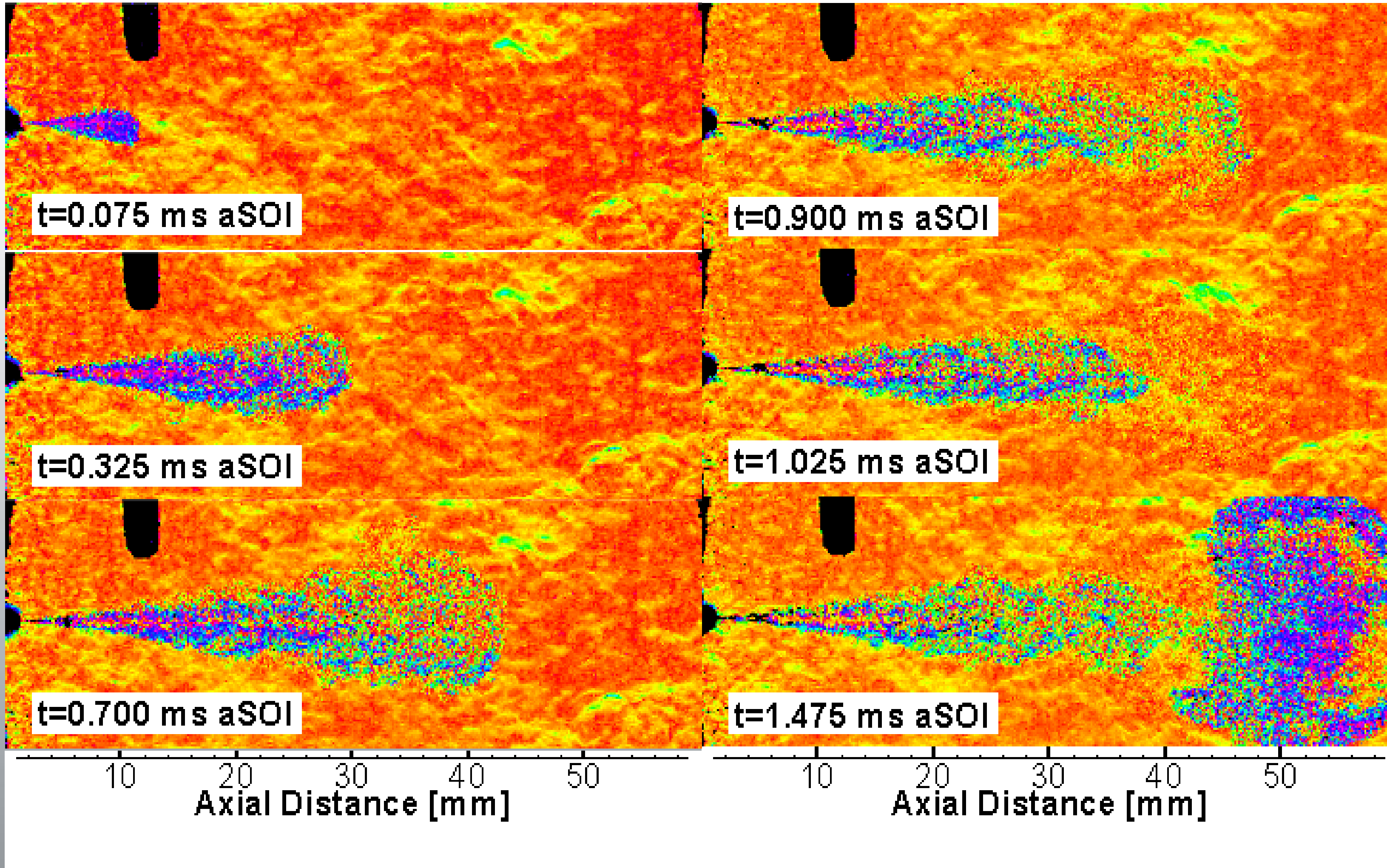
Here transverse displacement d(x,t) is related to hue or color

Rainbow Filter Calibration

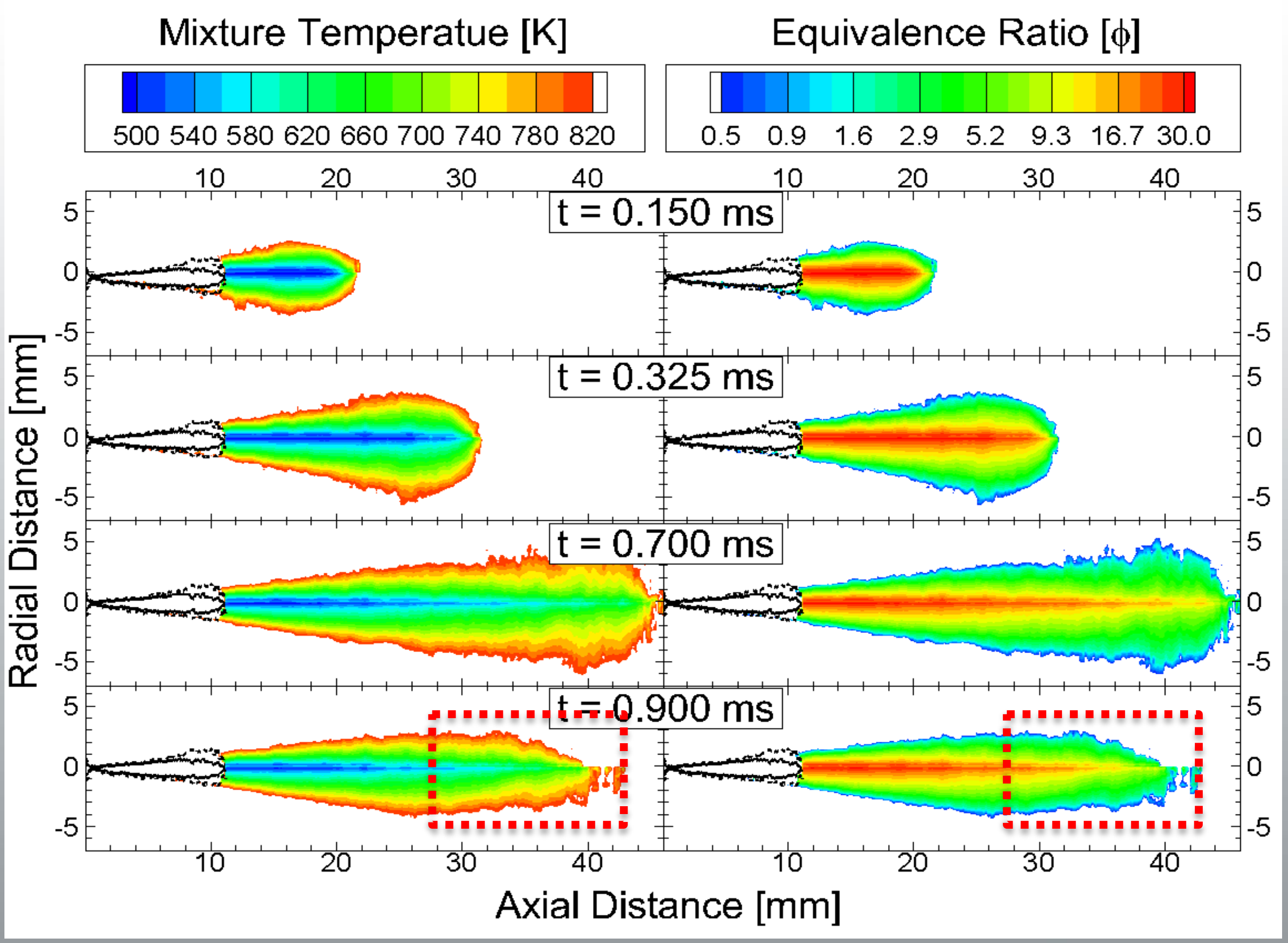


- Deflected rays pass through different colors on the filter.
- Filter serves as a ruler to measure the deflection of light rays, which is related to density or equivalence ratio.

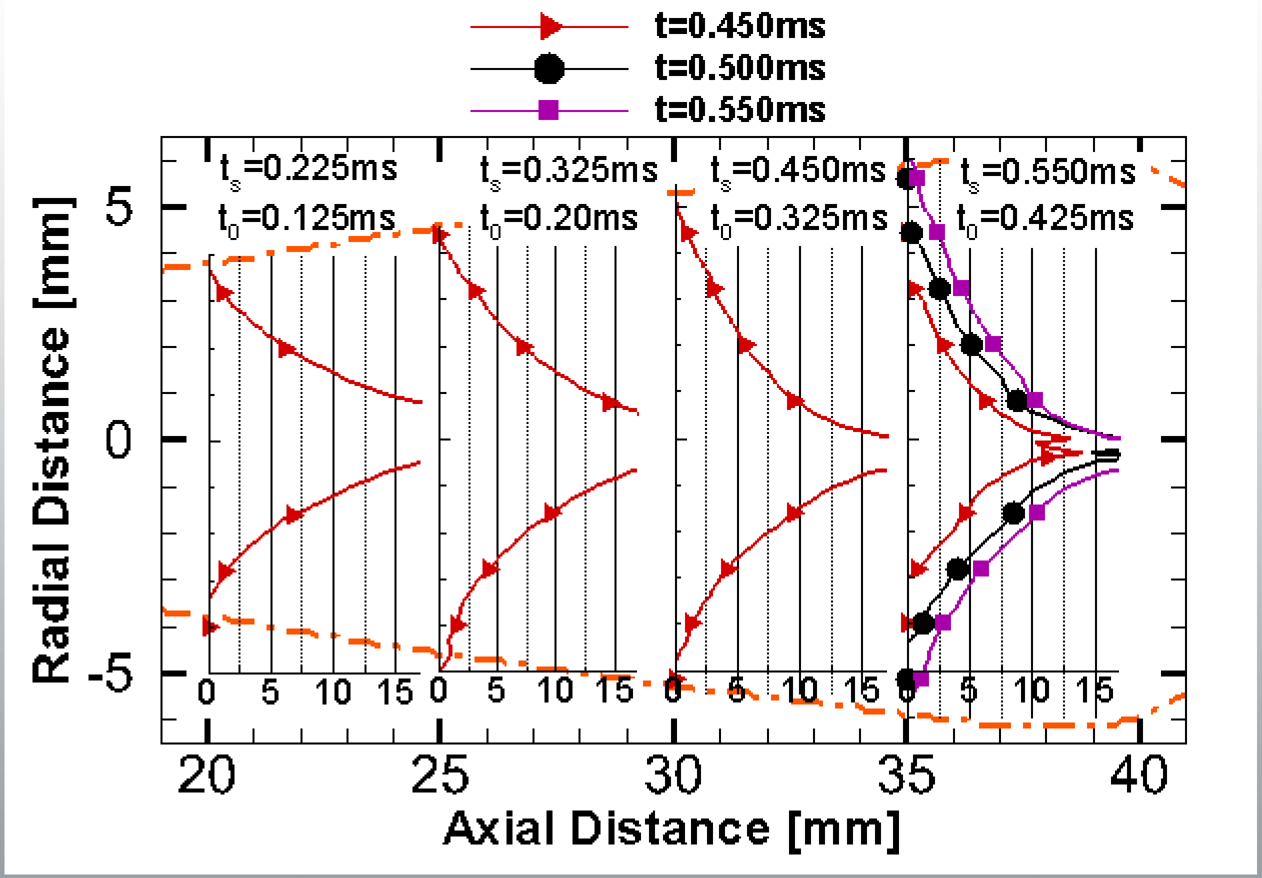
Rainbow Schlieren Images



Time Evolution



Radial Profiles



Integrated Diagnostics Setup

Additional Diagnostics include:

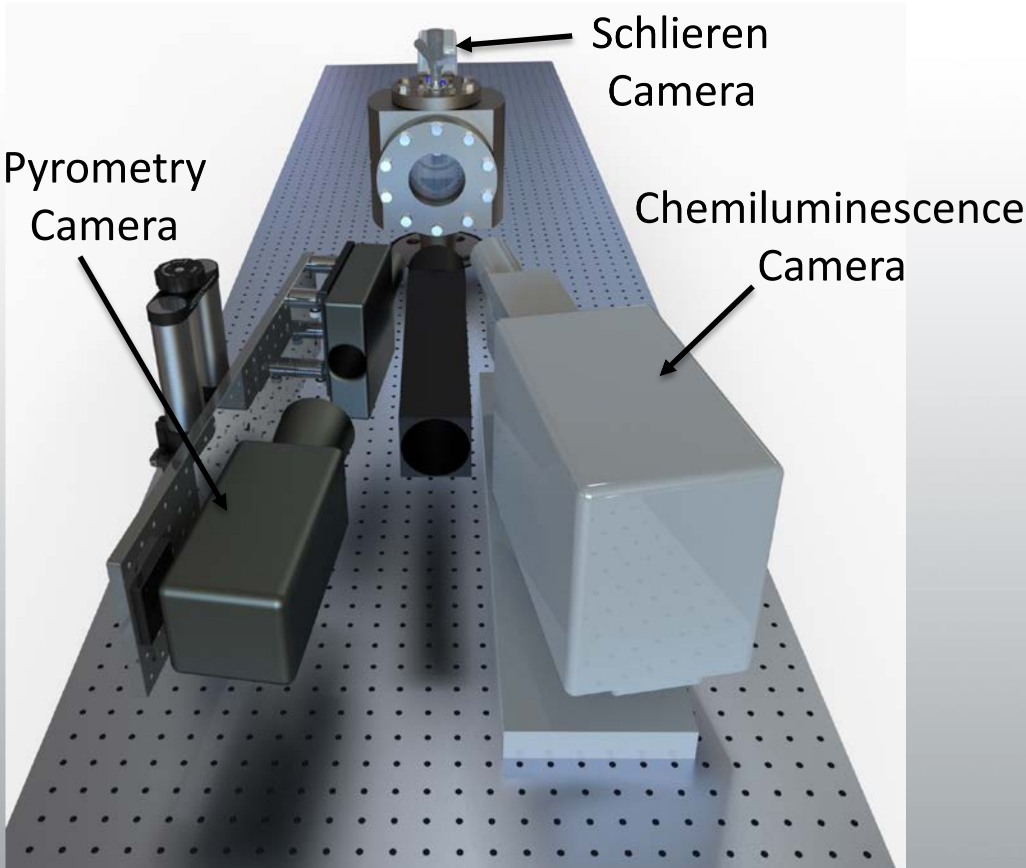
Two-color soot pyrometry

OH* Chemiluminescence

All three diagnostics have been integrated and synchronized by imaging a simple methane Bunsen burner flame.

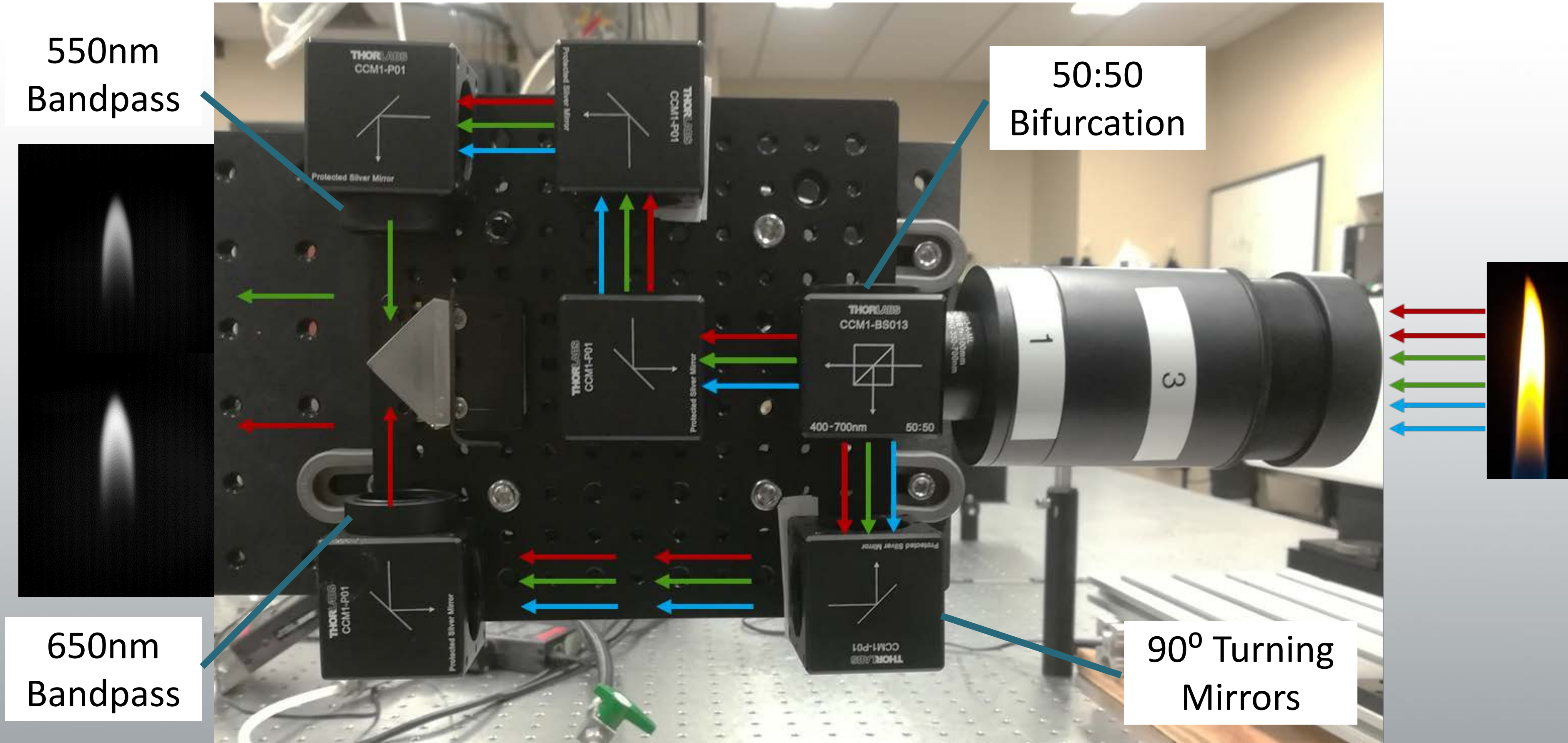
The integrated systems is now ready for use with CFPR.

Integrated Diagnostics Setup



– The Pyrometer and Chemiluminescence camera are set at angles on either side of the Schlieren light source

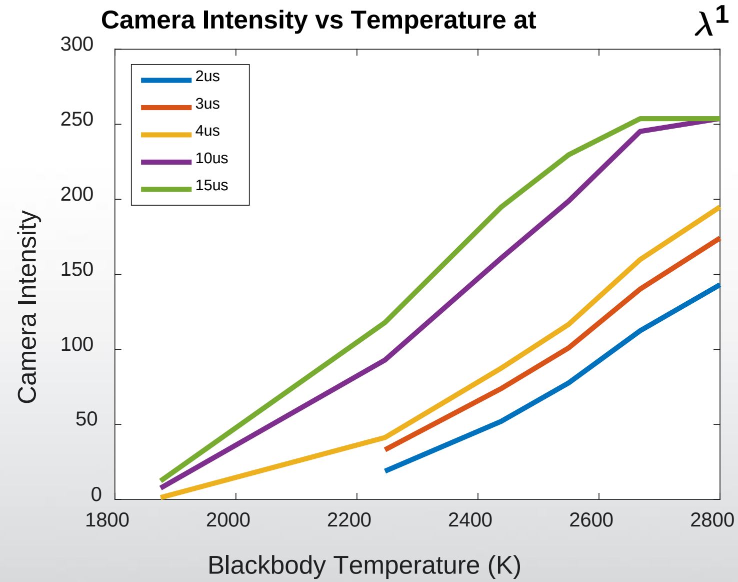
Two-Color Pyrometry

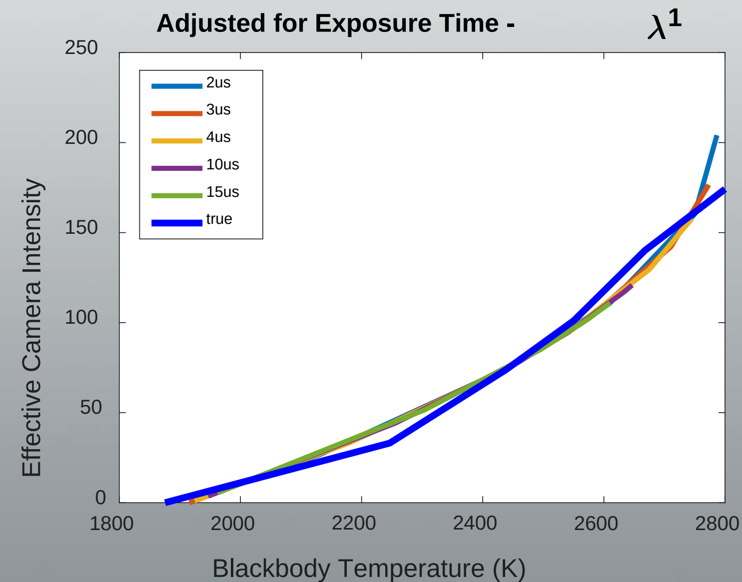


Radiation from the flame passes through a 50-50 beam splitter, a series of mirrors, and bandpass filters to yield an image on the camera sensor at each wavelength

Two-Color Pyrometry Principles

- Planck's Law: $E_{b,\lambda} = \dfrac{C_1}{\lambda^5\left[e^{\left({C_2}/{\lambda T}\right)}-1\right]}$
- Emissivity for a non-blackbody:
$$E_\lambda(T) = \epsilon_\lambda E_{b,\lambda}(T) = E_{b,\lambda}(T_a)$$
- Empirical relationship for emissivity[1]:
$$\epsilon_\lambda = 1 - e^{-KL/\lambda^\alpha}$$
- Combining:
$$\left[1-\left(\frac{e^{(C_2/\lambda_1 T)}-1}{e^{(C_2/\lambda_1 T_{a_1})}-1}\right)\right]^{{\lambda_1}^\alpha} = \left[1-\left(\frac{e^{(C_2/\lambda_2 T)}-1}{e^{(C_2/\lambda_2 T_{a_2})}-1}\right)\right]^{{\lambda_2}^\alpha}$$
    - T_{a1} and T_{a2} are measured, solve for T
- Calibrate camera signal to T_a with a known blackbody
- Use exposure constant to utilize full dynamics of the camera: $I_{eff} = {I_{rec}}/{C_{exp}}$





[1] Hottel & Broughton

OH* Chemiluminescence

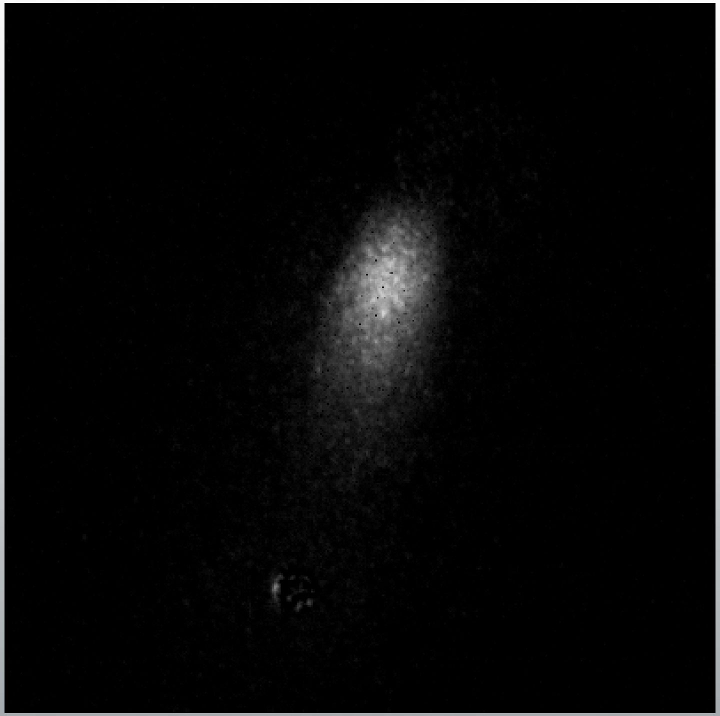
Photron FASTCAM SA5

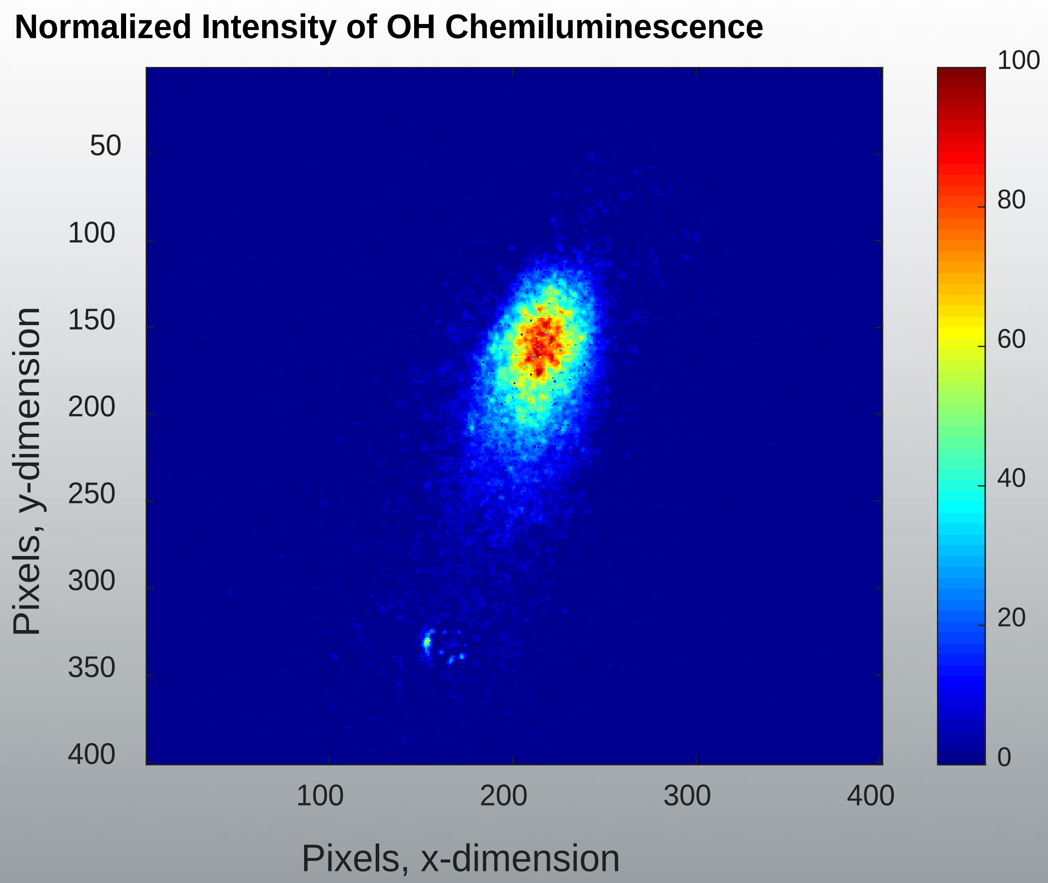
Invisible Vision UVi Camera Intensifier

315nm Single-Band Band Pass Filter

OH* Chemiluminescence

Steady CH_4 Flame Test

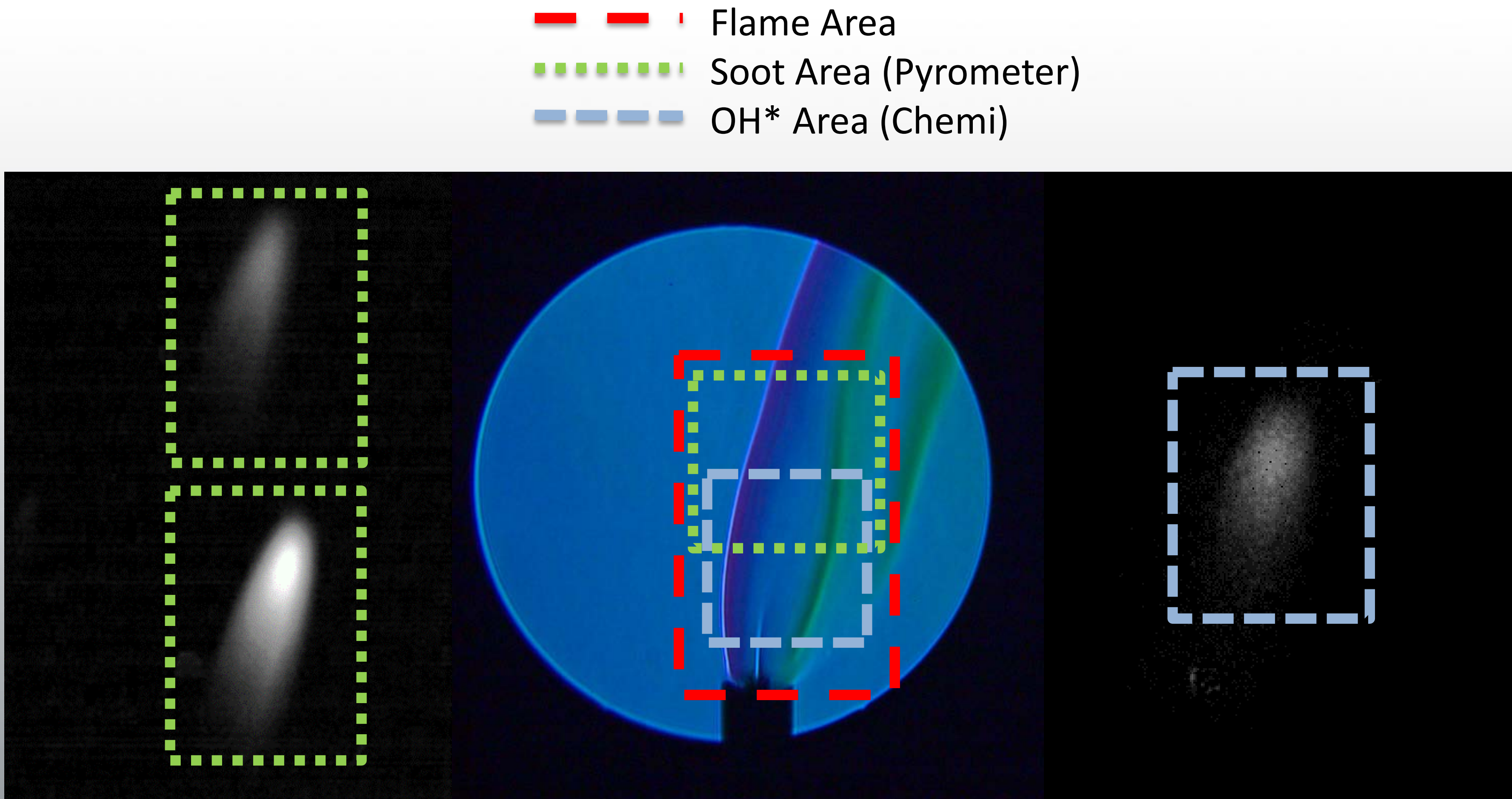




- 100 FPS
- Gate Time:100 µs
- Gain: 50%
- Cropped Resolution: 297x301
- Recorded Resolution: 1024x1024

Synchronized Image Acquisition

Steady CH_4 Flame Test



Two-Color Pyrometry | Rainbow Schlieren Deflectometry | OH* Chemiluminescence

Model Development Progress

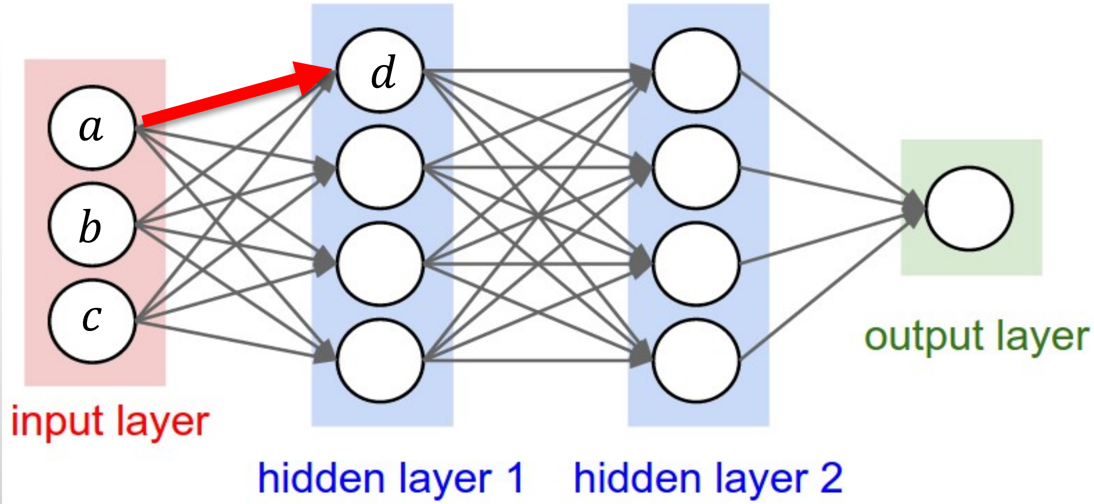
We quickly decided to pursue a neural network type model. Ultimate goal will be to develop model of the general form:

$$Combustion\ Properties\ = f\begin{pmatrix} Fuel\ Properties \\ Injection\ Properties \\ Ambient\ Properties \end{pmatrix}$$

To that end we have done initial exploration and proof of concept by developing a neural network that can replicate the predictions of the Siebers Liquid Length Model.

This network has been developed with the full set of Engine Combustion Network data that included liquid length.

Neural Network Structure

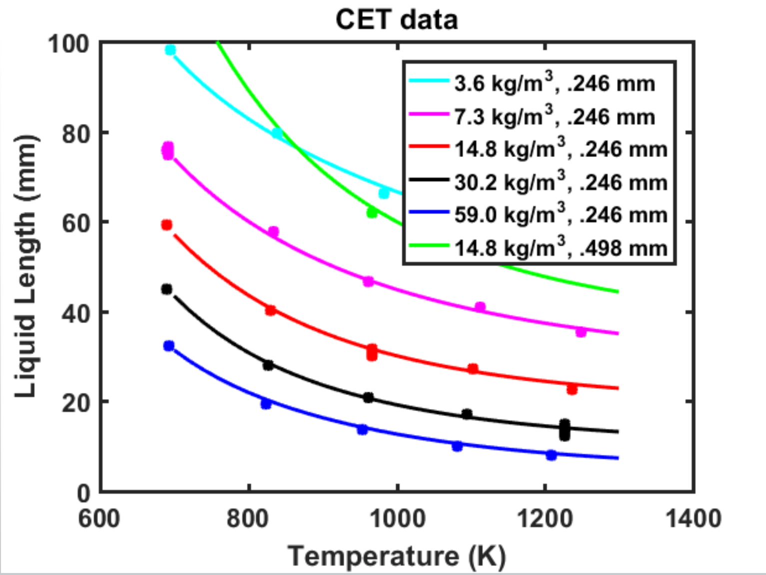


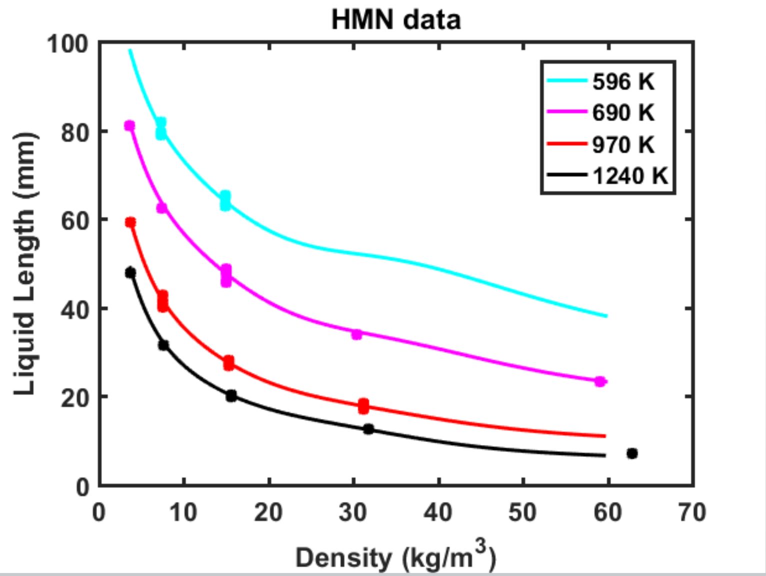
Equation for each connection: $d = \dfrac{2}{1 + e^{-2(G + W_1 a + W_2 b + W_3 c)}} - 1$

Terminology

- **Input Layer:** Each node represents raw data for an independent variable
- **Hidden Layers:** Node values are calculated based on the previous layer
- **Output Layer:** Nodes in the output layer represent the dependent variables
- **Connections and Weights:** Nodes are connected to each node in the subsequent layer via an activation function with a weight (W) and offset (G)
- **Activation Function:** The activation function for a connection defines the response of the second node in the connection to a change in the first node in the connection

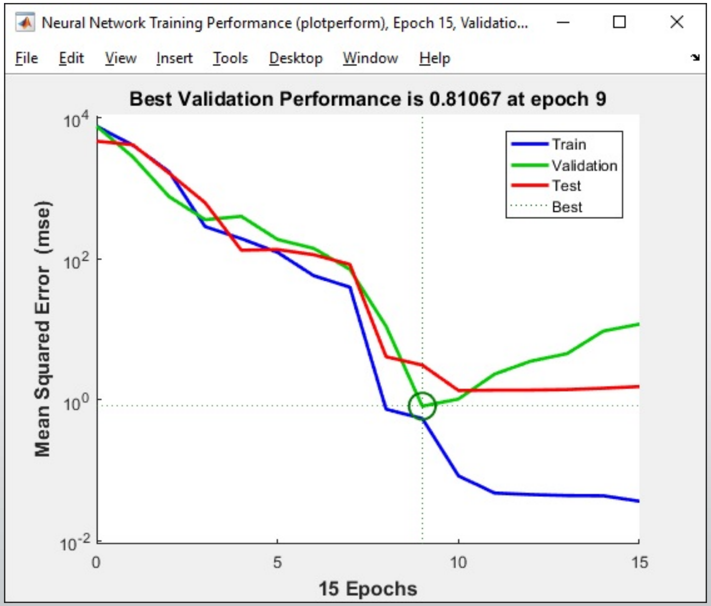
Neural Network Implementation

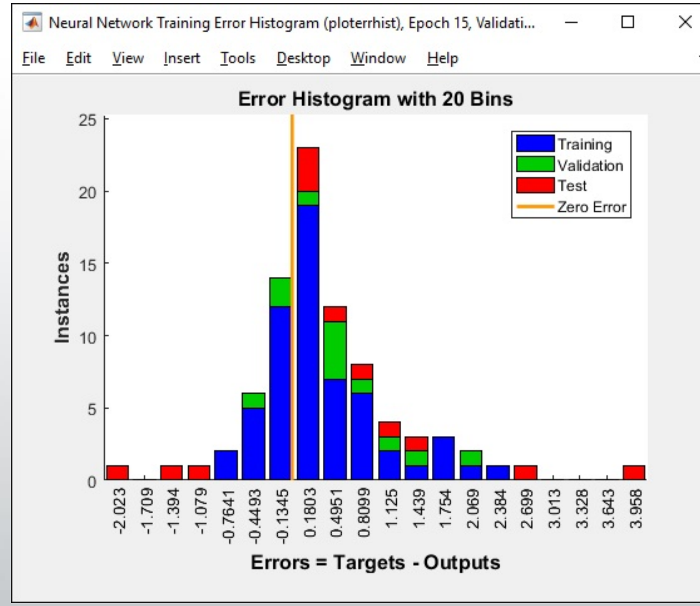




- Matlab neural network toolbox allows fast training with flexible network structure
- Proof-of-concept tests were conducted using ECN data to predict liquid length from bulk density, bulk temperature, fuel density, and nozzle diameter
- Unnecessarily complex network structures were found to produce unwanted behavior between data-dense areas in graphs
- Through trial and error, a network structure of two hidden layers with six nodes each was found to work best during this initial exploration.

Neural Network Training





– Experimental variation in data can cause non-physical behavior in the network, known as overfitting
– 15% of data is set aside for validation, and 15% for testing
– The network is trained on the remaining 70% of the dataset, and stops when it no longer improves for the validation data
– The test data is used to check for excessive error

Remaining Challenges and Barriers

- Identified potential fuel properties to test for relation to combustion properties. This includes supercritical fuel property effects.
- Spray tests of single component fuels will be completed to support model development
- Based on fuel properties and combustion properties an initial model structure will be completed
- Models for single component petroleum based fuels will be created
- Combustion properties that change non-linearly will be identified for more complex modeling development
- Model will be developed for predicting non-linear properties for fuel blends
- Blended fuels property models validated with acceptable accuracy

Proposed Future Research

- Conduct preliminary and baseline experiments in the modified CPFR
- Conduct parametric experimental study
- Evaluate the proposed EE approach with real-fluid model using an open source CFD code
- Evaluate the proposed EE approach with real-fluid model using a commercial CFD code
- Integrate the developed models into a commercial CFD code and perform validation and demonstration studies
- Document and disseminate validated source codes

Summary

Relevance

- This project will acquire experimental data, and develop property models to accuracy model fuel-air mixing at supercritical conditions for diesel application using open source and commercial CFD codes

Approach

- Innovative rainbow schlieren deflectometry optical diagnostics technique is used to acquire quantitative data in a constant pressure flow rig
- Detailed models to calculate thermodynamic properties are developed and implemented in CFD software, and validated.

Technical Accomplishments

- Developed and validated fluid property models using NIST database
- Identified test case, and coordinated to implement property models in CFD code
- Designed and constructed a constant pressure flow rig
- Implemented and validated schlieren diagnostics techniques

Future Work

- Implement property models in CFD software
- Acquire test data in the flow rig
- Compare experimental and model results to resolve any discrepancies
- Conduct parametric analysis

Collaboration and Coordination

- This projects builds on expertise in high speed diagnostics and experimental capabilities at The University of Alabama.
- UA is providing expertise in two areas:
  – Experimentation and optical diagnostics in a constant pressure flow rig
  – Neural network models to predict combustion properties
- As part of Co-optima project we partner with Sandia National Lab.
  – Partnership with Chuck Mueller to enable fuel selection and coordinate experiments activities.
  – We consult with both Chuck Mueller and Lyle Pickett to ensure safe and reliable operation of the test chamber.
  – Engagement with ECN
- Additional collaboration with Sibendu Som (Argonne) to support prediction and validation of computational fluid dynamics models.
- UA Investigators hold weekly meetings with students to guide their efforts and work directly with students to ensure rigorous treatment of all aspects of the project.

Remaining Challenges and Barriers

- Identify potential fuels and fuel properties for experiments.
- Determine key combustion properties based on experiments
- Conduct experiments over a range of test conditions
- Develop reliable neural network model structure and models for
  - single component fuels
  - Multi-component fuels
- Blended fuels property models validated with acceptable accuracy would be a challenge

Proposed Future Research

- Conduct preliminary and baseline experiments using the three diagnostics techniques simultaneously.
- Post-process experimental results to obtain combustion properties of relevance for single component fuels (both petroleum- and bio-based fuels).
- Develop neural network models to relate fuel and combustion properties.
- Conduct experiments to obtain combustion properties for multi-component fuels.
- Extend and validate neural network models for multi-component fuels.
- Disseminate experimental results and models.

Summary

Relevance

- This project will provide experimental data, and develop combustion property prediction models to support larger Co-Optima effort of targeting fuels that promote specific combustion relevant outcomes (i.e. low soot, etc.)

Approach

- Rainbow schlieren deflectometry (RSD), two-color pyrometry, and OH* chemiluminescence optical diagnostics techniques are used with high temporal resolution to acquire quantitative mixing, ignition, and soot measurements in a constant pressure flow rig (CPFR)
- Neural Network (NN) models are used to predict combustion properties for different fuels, injection, and ambient conditions.

Technical Accomplishments

- Acquired RSD measurements in a reacting fuel spray at diesel conditions.
- Developed a two-color (2C) pyrometer system and calibration methods.
- Integrated RSD, OH* chemiluminescence, and two-color pyrometer for simultaneous image acquisition.
- Developed proof of concept for NN models to predict liquid length using ECN database.

Future Work

- Complete baseline testing and synchronous image acquisition with 3 diagnostics techniques using CPFR.
- Formalize data aggregation methods.
- Complete parametric fuels testing
- Complete model development

Technical Backup Slides

Time Averaging

Average transverse deflection angle is related to average refractive index gradient

$$\varepsilon(x,t) = \int \frac{\partial \delta}{\partial x}(x,y,t)dy$$

$$\varepsilon(x,t) = \bar{\varepsilon}(x) + \varepsilon'(x,t)$$

$$\delta(x,y,t) = \bar{\delta}(x,y) + \delta'(x,y,t)$$

$$\bar{\varepsilon}(x) + \varepsilon'(x,t) = \int \frac{\partial}{\partial x}\left(\bar{\delta}(x,y) + \delta'(x,y,t)\right)dy$$

$$\overline{\bar{\varepsilon}(x) + \varepsilon'(x,t)} = \int \overline{\frac{\partial}{\partial x}\left(\bar{\delta}(x,y) + \delta'(x,y,t)\right)}\, dy$$

$$\overline{\varepsilon'(x,t)} = 0 \qquad \overline{\delta'(x,y,t)} = 0$$

$$\bar{\varepsilon}(x) = \int \frac{\partial}{\partial x}\left(\bar{\delta}(x,y)\right)dy$$

Determination of Local Properties

Starting with

$$\bar{\varepsilon}(x) = \int \frac{\partial}{\partial x}\left(\bar{\delta}(x,y)\right)dy$$

and, after conversion to radial coordinates and Abel inversion gives a solution for $\bar{\delta}$ as

$$\bar{\delta}(r) = \frac{-1}{\pi}\int_r^R \bar{\varepsilon}(x)\frac{dx}{\sqrt{x^2 - r^2}}$$

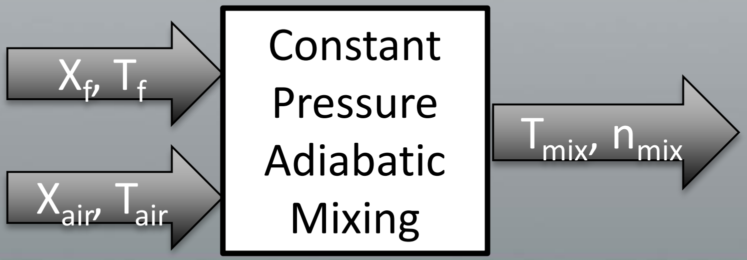
which can be discretized to

$$\bar{\delta}(r_i) = \sum D_{ij}\,\bar{\varepsilon}_j$$

For a mixture of gases (vapor region), refractive index is sum of the product of all species Gladstone-Dale constant and partial density.

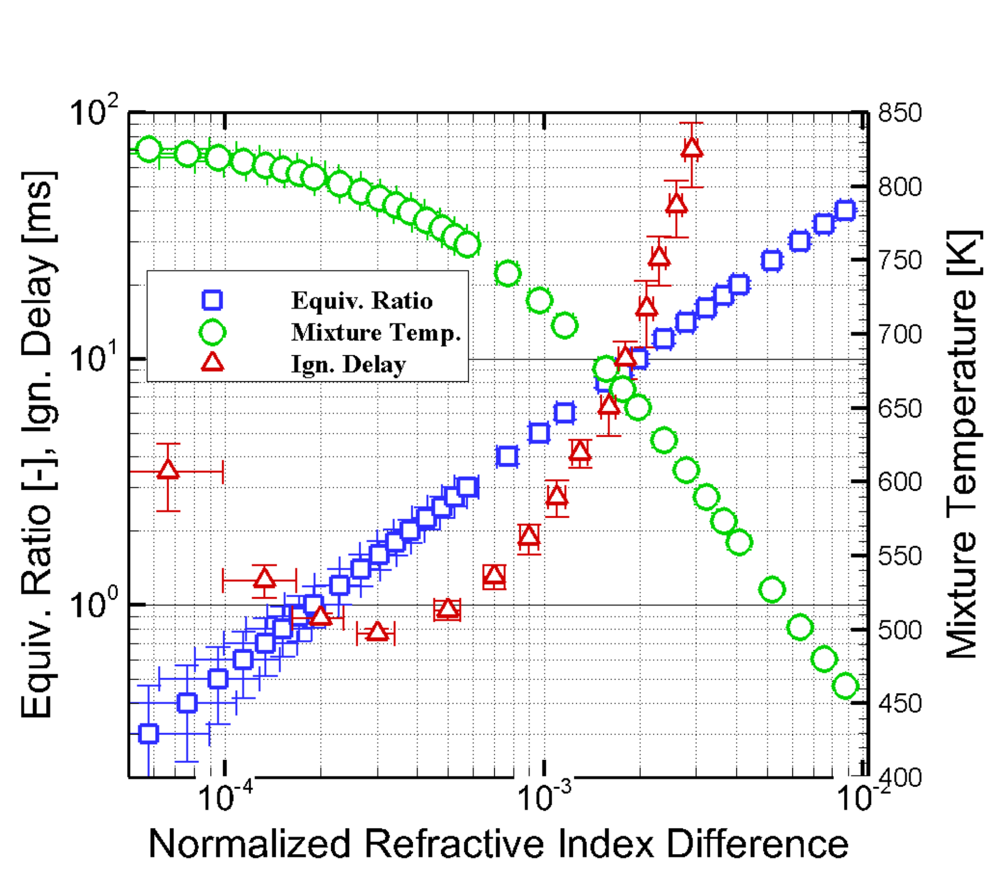
$$n = n_o(\delta + 1) = \sum_i \kappa_i \rho_i = \kappa_{air}\frac{P_{air}x_{air}}{R_{air}T_{mix}} + \kappa_f \rho_f$$

- Mixture refractive index is a unique function of mixture fraction and temperature
- Determined based on a simple adiabatic mixing (no chemistry) model.



Determination of Local Properties

- An indication of mixture ignitability is considered from simple PSR simulations at pairs of ϕ,T_{mix}.
- For a measured refractive index difference, corresponding local properties are interpolated.
- Uncertainties currently based on simplified propagation of image hue to refractive index



Results at 0.7ms aSOI